Entropies based on fractional calculus

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Abstract

We propose entropy functions based on fractional calculus. We show that this new entropy has the same properties than the Shannon entropy except additivity. We show that this entropy function satisfies the Lesche and thermodynamic stability criteria.

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1 Introduction

In the last two decades, there has been a lot of interest in generalizing the Shannon entropy and exploring the consequences of applying these new entropies to physics and other fields. These entropy functions depend on an additional parameter q and become the Shannon entropy function when this parameter takes the value $q = 1$. The implications of these generalizations are not merely mathematical but in some cases these entropies could be non-extensive opening the possibility for applications to systems with long range correlations.

The most studied generalization of the Shannon entropy, besides the Rényi entropy [1], is the Tsallis entropy [2]

$$S_q = \frac{k}{q-1}\left(1 - \sum_i p_i^q\right), \tag{1}$$

where p_i is the probability . The probability distribution under the constraints $\sum_i p_i = 1$ and $\sum p_i \epsilon_i = E$ is given by the function

$$p_i = \frac{[1-\beta(q-1)\epsilon_i]^{1/(q-1)}}{Z_q}, \tag{2}$$

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where Z_q is the partition function. Many applications of this entropy can be found in the literature, not only in statistical mechanics but also in other fields like economics, biology, gravitation and high energy collisions [3].

More recently, another non-additive entropy was proposed [4][5] according to the function

$$S(q) = -\sum_i p_i^q \ln p_i, \tag{3}$$

leading to the probability distribution

$$p_i = \left(\frac{-qW(z)}{(a+bE)(q-1)} \right)^{1/(1-q)}, \tag{4}$$

where the variable z is a function of the energy E and the parameter q, and $W(z)$ is the Lambert function [6] defined by

$$W(z)e^{W(z)} = z \tag{5}$$

In addition, with use of optimization principles, several other entropies (or measures) have been proposed [7][8] to address issues in information theory. One of these measures, is the Havrada-Charvat measure given by the function

$$S(p:q) = \frac{\sum_i p_i^\alpha P_i^{1-\alpha} - 1}{\alpha - 1}, \tag{6}$$

which is a relative entropy that becomes the Kullback-Liebler measure for $\alpha = 1$ and the Tsallis entropy for $P_i = 1$.

In particular, in statistical mechanics, the main motivation to propose new entropies resides in the hope that they could describe phenomena that lie outside the scope of the Boltzmann-Gibbs formalism.

This paper is organized as follows. In Section 2 we give a brief description of fractional derivatives. In Section 3 with use of the fractional derivative we define the new entropy, and maximize it subject to the constraint equations $\sum_i p_i = 1$ and $\sum p_i \epsilon_i = E$, and find that the probability distribution has an exponential solution for $q = 1/2$. In Section 4 we study two criteria of stability of this entropy function, and in Section 5 we summarize our results.

2 Fractional Derivatives

The subject of fractional calculus is one of the many examples of a mathematical formalism that, in spite of its long history, it has remained until recently practically absent in the physics literature. L'Hopital in 1695 wondered about the meaning of $\frac{d^m f(x)}{dx^m}$ for $m = 1/2$, and it was until the first half of the nineteen century that a precise mathematical formulation of fractional calculus was developed thanks to the contributions of mathematicians like N. H. Abel, J. B. Fourier, J. Liouville and B. Riemann, among many others [9]. More recently, some applications of fractional calculus include the fields of anomalous diffusion, chaos, polymer science, biophysics, and field theory [10]-[13]. The idea

behind the definition of a fractional derivative resides in finding an operator that generalizes the equation

$$\frac{d^n x^m}{dx^n} = \frac{m!}{(m-n)!} x^{m-n}, \tag{7}$$

for arbitrary $n \in R^+$, by replacing each factorial by a gamma function

$$\frac{d^q x^\mu}{dx^q} = \frac{\Gamma(\mu+1)}{\Gamma(\mu-q+1)} x^{\mu-q} \qquad , q > 0. \tag{8}$$

This generalization is fulfilled by defining the operator

$$_aD_t^q = \left(\frac{d}{dt}\right)^n ({}_aD_t^{q-n} f(t)), \tag{9}$$

where $n \in N$, $n > q$ and

$$_aD_t^{q-n} f(t) = \frac{1}{\Gamma(n-q)} \int_a^t \frac{f(t')}{(t-t')^{(1+q-n)}} dt'. \tag{10}$$

Equation (10) defines the fractional integral operator. There is also a right Riemann-Liouville derivative, which plays an important role in integration by parts and it is defined according to

$$_tD_b^q = \left(-\frac{d}{dt}\right)^n ({}_tD_b^{q-n} f(t)), \tag{11}$$

with

$$_tD_b^{q-n} f(t) = \frac{1}{\Gamma(n-q)} \int_t^b \frac{f(t')}{(t-t')^{(1+q-n)}} dt'. \tag{12}$$

3 Entropy Functions

The observation that the Shannon entropy can be defined from the equation

$$S = \lim_{t\to -1} \frac{d}{dt} \sum_i p_i^{-t}, \tag{13}$$

opened the possibility to define new entropy functions. In particular, it was pointed out [14] that the Tsallis entropy can be expressed in an equivalent way as [1]

$$S = \lim_{t\to -1} D_q^t \sum_i p_i^{-t}, \tag{14}$$

where the operator D_q^t is called the Jackson [15] q-derivative defined as

$$D_q^t = t^{-1} \frac{1 - q^{td/dt}}{1-q}. \tag{15}$$

[1]Our Eq. (14) is slightly different than the one proposed by S. Abe.

Since the Jackson derivative plays an important role in the formulation of non-commutative calculus and thus in quantum groups, it is expected [16] that quantum groups may also play an important role in Tsallis formalism. Other entropy functions have been defined with the use of variations of the Jackson q-derivative [17][18], a new thermostatistics based on q-analysis [19] and generalizations of the Tsallis entropy [20].

Here we use the same approach as in Equation (14) but with the operator defined in Eq. (10) with $a = -\infty$. Therefore our entropy is given by the equation

$$S_q[p] = \lim_{t\to -1} \frac{d}{dt}\left({}_{-\infty}D_t^{q-1} \sum_i e^{-t\ln pi} \right), \tag{16}$$

where $0 \leq q \leq 1$. Therefore, we need to solve the following integral

$$S_q[p] = \lim_{t\to -1} \frac{d}{dt}\frac{1}{\Gamma(1-q)} \sum_i \int_{-\infty}^{t} \frac{e^{-t'\ln p_i}}{(t-t')^q} dt'. \tag{17}$$

By defining a new variable $w = t - t'$ and with use of the definition of the $\Gamma(z)$ function

$$\Gamma(z) = x^z \int_0^\infty t^{z-1} e^{-tx} dt \quad x > 0\ ,\ z > 0 \tag{18}$$

we find, after taking the ordinary derivative and setting $t = -1$, that the entropy becomes the function

$$S_q[p] = \sum_i (-\ln p_i)^q p_i. \tag{19}$$

It is clear that $S[q] = \sum_i s_i(p)$ is positive, and from the condition $\frac{\partial s_i(p)}{\partial p_i} = 0$ we see that $s_i(p)$ has a maximum at $p_i = e^{-q}$ with a second derivative at this point given by $\frac{\partial^2 s_i(p)}{\partial p_i^2} \mid_{p_i=e^{-q}} = -q^{q-1}e^q$. This maximum will be closed to $p \approx 1$ for $q \approx 0$ and close to $p \approx 0$ for $q \gg 1$. In particular, the binary entropy

$$S_q^{bin} = p(-\ln p)^q + (1-p)(\ln(1-p))^q, \tag{20}$$

has a maximum at $p = 1/2$. In addition, as expected, this entropy is non-additive. Let $\mathbf{p} = (p_1, ..., p_m)$ and $\mathbf{P} = (P_1, ..., P_n)$ be two independent probability distributions for systems A and B respectively. The entropy for the joint probability is given by

$$S_q[A, B] = \sum_{i=1}^{m} \sum_{j=1}^{n} p_i P_j \left(-\ln(p_i P_j)\right)^q. \tag{21}$$

A simple calculation shows that Eq. (21) becomes the infinite series

$$S_q[A, B] = S_q[A] + \sum_{i=1}^{m} \sum_{j=1}^{n} \sum_{k=1} \binom{q}{k} p_i P_j (-\ln p_i)^k (-\ln P_j)^{q-k}, \tag{22}$$

such that exchanging $P \leftrightarrow p$ we can symmetrize this equation leading to

$$S_q[A,B] = \frac{1}{2}\left\{S_q[A] + S_q[B] + \sum_{k=1} \tbinom{q}{k} \left[S_k[A]S_{q-k}[B] + S_{q-k}[A]S_k[B]\right]\right\}. \tag{23}$$

A simple check shows that we recover the additive property by taking the $lim_{q\to 1}S_q[A,B]$ where $S_0[p] = 1$ and $S_1[p] = S_{Shannon}$.

As is well known, the probability distributions can be obtained by maximizing the corresponding entropy function subject to some constraint equations. Therefore, we need to maximize

$$L = S_q[p] + \alpha\left(1 - \sum_i p_i\right) + \beta\left(E - \sum_i p_i\epsilon_i\right), \tag{24}$$

such that setting $\frac{dL}{dp_j} = 0$, leads to the equation

$$(-\ln p_j)^q - q(-\ln p_j)^{q-1} = \alpha + \beta\epsilon_j. \tag{25}$$

For the particular case of $q = 1/2$ there is an exact solution to Eq. (25) with

$$p \propto e^{(-1/2)(\Omega^2 + \sqrt{\Omega^2+2}\,\Omega)}, \tag{26}$$

where $\Omega = \beta\epsilon + \alpha$.

4 Stability

In this section we investigate the stability properties of the new entropy for the cases of Lesche and thermodynamic stability criteria.

4.1 Lesche stability

In a seminal article [21][22] Lesche proposed a stability criterion to study the stability of the Rényi entropy function. He showed that the Rényi entropy is unstable for every value of the q parameter with the exception of $q = 1$. Therefore, under this stability criterion the Shannon entropy is stable. The main motivation of this type of stability is to check whether an observable changes appreciably when the probability assignments p on a set of n microstates is perturbed by an infinitesimal amount δp. This criteria has already been applied [23]-[26] to some generalizations of the Shannon entropy. Let p and p' be two probability assignments, Lesche stability requires that $\forall\epsilon > 0$ we can find a $\delta > 0$ such that

$$\sum_{j=1}^{n} |p_j - p'_j| \leq \delta \Longrightarrow \frac{|S_q[p'] - S_q[p]|}{S_q^{max}} < \epsilon. \tag{27}$$

Starting from Eq. (27) and an expression for a generalized entropy maximized by a probability distribution, the authors of [24] derived a simple condition from which Lesche stability can be addressed. In Ref. [24] it is shown that Lesche stability is satisfied if

$$\frac{|S_q[p'] - S_q[p]|}{S_q^{max}} < C \sum_{j=1}^{n} |p_j - p'_j|, \tag{28}$$

where the constant C is given by

$$C = \frac{f^{-1}(0^+) - f^{-1}(1^-)}{f^{-1}(0^+) - \int_0^1 f^{-1}(t)dt}, \tag{29}$$

and the function $f^{-1}(t)$ is the inverse of the probability distribution. Therefore if $C \neq 0$, we can take an arbitrary δ as $\delta = \epsilon/C$ such that the criterion in Eq. (27) is fulfilled. From Eq. (25) we see that in our case

$$f^{-1}(t) = (-\ln t)^q - q(-\ln t)^{q-1}, \tag{30}$$

such that replacing in Eq. (29) we obtain

$$C = \lim_{t \to 0^+} \frac{f^{-1}(t)}{f^{-1}(t) - \Gamma(1+q) + q\Gamma(q)} = 1, \tag{31}$$

and taking $\delta = \epsilon$ the inequality in Eq. (28) is satisfied and thus Eq. (27).

4.2 Thermodynamic stability

As is well known, in the Boltzmann-Gibbs formalism the concavity of the entropy, $\frac{\partial^2 S}{\partial U^2} < 0$, is equivalent to the condition of thermodynamic stability. It has been recently shown [25] that for the case of a non-additive entropy the property of concavity does not imply thermodynamic stability. The study of thermodynamic stability of some non-additive entropies can be found in [25][26][27]. Given an isolated system composed of two independent and identical subsystems in equilibrium in which there is a small amount of internal energy transfered from one to the other, the property $\frac{\partial^2 S_q}{\partial U^2} < 0$ does not necessarily implies that

$$S_q(U,U) > S_q(U + \Delta U, U - \Delta U), \tag{32}$$

provided that the initial state is a state that maximizes the total entropy. Inserting Equation (23) into Equation (32) and expanding up to $(\Delta U)^2$ after some algebra we find

$$0 > \frac{1}{2} S''_q + \sum_{k=1}^{\infty} \binom{q}{k} \left(\frac{1}{2}(S_{q-k}S''_k + S''_{q-k}S_k) - S'_k S'_{q-k} \right). \tag{33}$$

In the microcanonical picture $S_q = \ln^q n$, and we can analyze the summation in Equation (33) by writing the functions S'_k and S''_k in terms of S_k as follows

$$\begin{aligned} S'_k &= \frac{k}{n} S_{k-1} \\ S''_k &= -\frac{k}{n^2} \left(S_{k-1} - (k-1) S_{k-2}\right) \\ S_k S_{q-k} &= S_q, \end{aligned} \tag{34}$$

such that replacing these identities into Equation (33) and performing the summations we find

$$0 > \frac{1}{2} S''_q - \frac{2^q - 1}{2n^2} \left(q S_{q-1} + (q - q^2) S_{q-2}\right), \tag{35}$$

which due to the fact that S_q is a positive and concave function Equation (35) satisfies the inequality for $0 < q < 1$ and therefore thermodynamic stability. A simple check shows that the condition $0 > S''(q)$ is recovered for $q = 1$.

5 Conclusions

In this paper we defined a new entropy function in the context of fractional calculus. This new entropy is concave, positive definite and non-additive. Maximizing the entropy subject to the usual constrains leads to an exponential probability distribution for $q = 1/2$. In addition, we have shown that this entropy satisfies Lesche and thermodynamic stability. There are several issues one could address regarding the proposed entropy. In order to determine whether the non-additive property of this entropy implies non-extensivity, it will require to compute within this framework the correlation function and correlation length for a simple ideal gas and compare them with the $q = 1$ case. For example, this type of calculation was performed in [28] to check the factorization approach [29] of Tsallis quantum statistics, and it was found that correlations are smaller for $q \neq 1$ putting into question the crude approximation used in Ref. [29]. In addition, it is an open problem in what type of applications could this entropy function be successfully used, particularly in those fields where the Shannon entropy have presented limitations, as for example in the formulation of algorithms for image segmentation [30]. We will attempt to address some of these questions in future communications.

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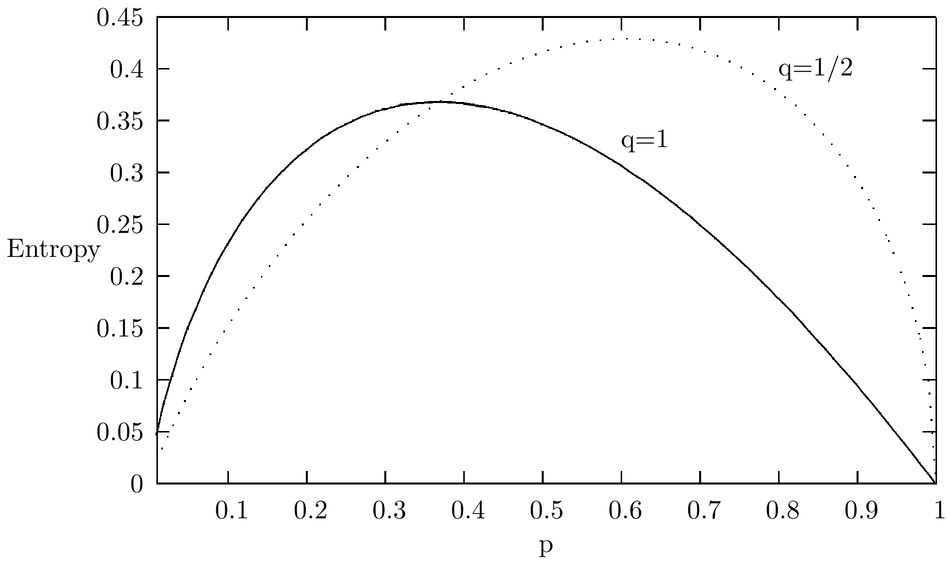
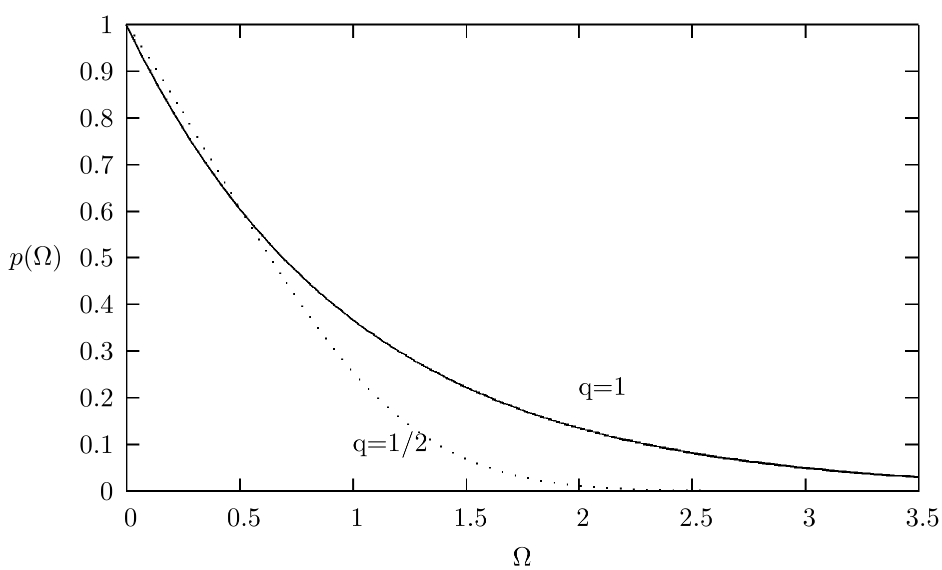
Fig. 1:The entropy function for $q = 1/2$ and the Shannon entropy ($q = 1$)

Fig. 2:The probability distribution $p(\Omega)$ for $q = 1/2$ and $q = 1$



0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
Entropy
0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1
p
q=1/2
q=1



1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
$p(\Omega)$
0 0.5 1 1.5 2 2.5 3 3.5
Ω
q=1
q=1/2